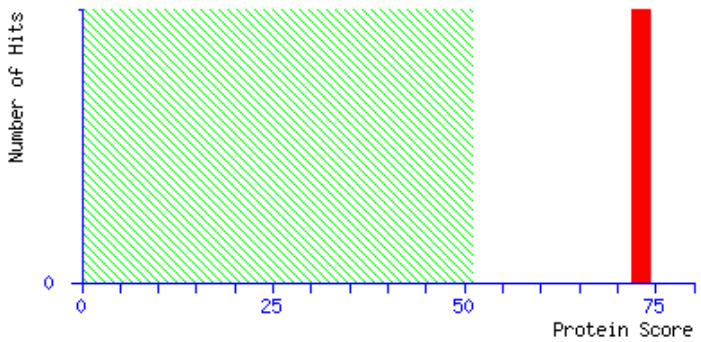
Mascot Search Results

```
User            : Lily-mascot
Email           : l.r.adair@pgr.reading.ac.uk
Search title    : Peptide mix chimeric MS/MS m/z 524 (03072023)
MS data file    : 524.txt
Database        : SwissProt 2021_01 (564277 sequences; 203340877 residues)
Taxonomy        : Eukaryota (eucaryotes) (192754 sequences)
Timestamp       : 3 Jul 2023 at 13:32:16 GMT
Protein hits    : COLI_BALBO Pro-opiomelanocortin (Fragment) OS=Balaenoptera borealis OX=9768 GN=POMC PE=1 SV=1
```

Mascot Score Histogram

Ions score is -10*Log(P), where P is the probability that the observed match is a random event.
Individual ions scores > 51 indicate identity or extensive homology (p<0.05).
Protein scores are derived from ions scores as a non-probabilistic basis for ranking protein hits.



Peptide Summary Report

Format As [Peptide Summary] Help

Significance threshold p< 0.05 Max. number of hits AUTO

Standard scoring ◉ MudPIT scoring ○ Display non-significant matches ☐ Show sub-sets 0

Show pop-ups ◉ Suppress pop-ups ○ Sort unassigned [Decreasing Score] Require bold red ☐

Preferred taxonomy [All entries]

Select All | Select None | Search Selected | ☐ **Error tolerant** | Archive Report

1. COLI_BALBO **Mass:** 4538 **Score:** 73 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin (Fragment) OS=Balaenoptera borealis OX=9768 GN=POMC PE=1 SV=1
☐ Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
☑ 2	2093.0862	2092.0789	2092.0789	0.03	0	73	0.00035	1	U	-.SYSMEHFRWGKPVGKKR.R

Proteins matching the same set of peptides:
COLI_BALPH **Mass:** 4538 **Score:** 73 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin (Fragment) OS=Balaenoptera physalus OX=9770 GN=POMC PE=1 SV=1
COLI_LOXAF **Mass:** 14925 **Score:** 73 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin (Fragment) OS=Loxodonta africana OX=9785 GN=POMC PE=1 SV=1
COLI_RABIT **Mass:** 4475 **Score:** 73 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin (Fragment) OS=Oryctolagus cuniculus OX=9986 GN=POMC PE=1 SV=1
COLI_CAVPO **Mass:** 28246 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Cavia porcellus OX=10141 GN=POMC PE=1 SV=2
COLI_LITCT **Mass:** 30370 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Lithobates catesbeianus OX=8400 GN=pomc PE=1 SV=1
COLI_MOUSE **Mass:** 26690 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)

Pro-opiomelanocortin OS=Mus musculus OX=10090 GN=Pomc PE=1 SV=1
COLI_NEOVI **Mass:** 15812 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin (Fragment) OS=Neovison vison OX=452646 GN=POMC PE=2 SV=1
COLI_PIG **Mass:** 28876 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Sus scrofa OX=9823 GN=POMC PE=1 SV=1
COLI_RAT **Mass:** 26523 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Rattus norvegicus OX=10116 GN=Pomc PE=1 SV=1
COLI_SHEEP **Mass:** 29043 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Ovis aries OX=9940 GN=POMC PE=1 SV=3
COLI_BOVIN **Mass:** 29242 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Bos taurus OX=9913 GN=POMC PE=1 SV=1
COLI_HUMAN **Mass:** 29405 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Homo sapiens OX=9606 GN=POMC PE=1 SV=2
COLI_MACNE **Mass:** 29153 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Macaca nemestrina OX=9545 GN=POMC PE=1 SV=2
COLI_PELRI **Mass:** 30049 **Score:** 71 **Matches:** 1(1) **Sequences:** 1(1)
Pro-opiomelanocortin OS=Pelophylax ridibundus OX=8406 GN=pomc PE=2 SV=1

Peptide matches not assigned to protein hits: (no details means no match)

	Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
☑	1	1046.5418	1045.5345	1045.5444	-9.43	0	25	20	1		VYPNIPKES

Search Parameters

```
Type of search         : MS/MS Ion Search
Enzyme                 : None
Mass values            : Monoisotopic
Protein Mass           : Unrestricted
Peptide Mass Tolerance : ± 10 ppm
Fragment Mass Tolerance: ± 0.2 Da
Max Missed Cleavages   : 0
Instrument type        : MALDI-QUAD-TOF
Number of queries      : 2
```

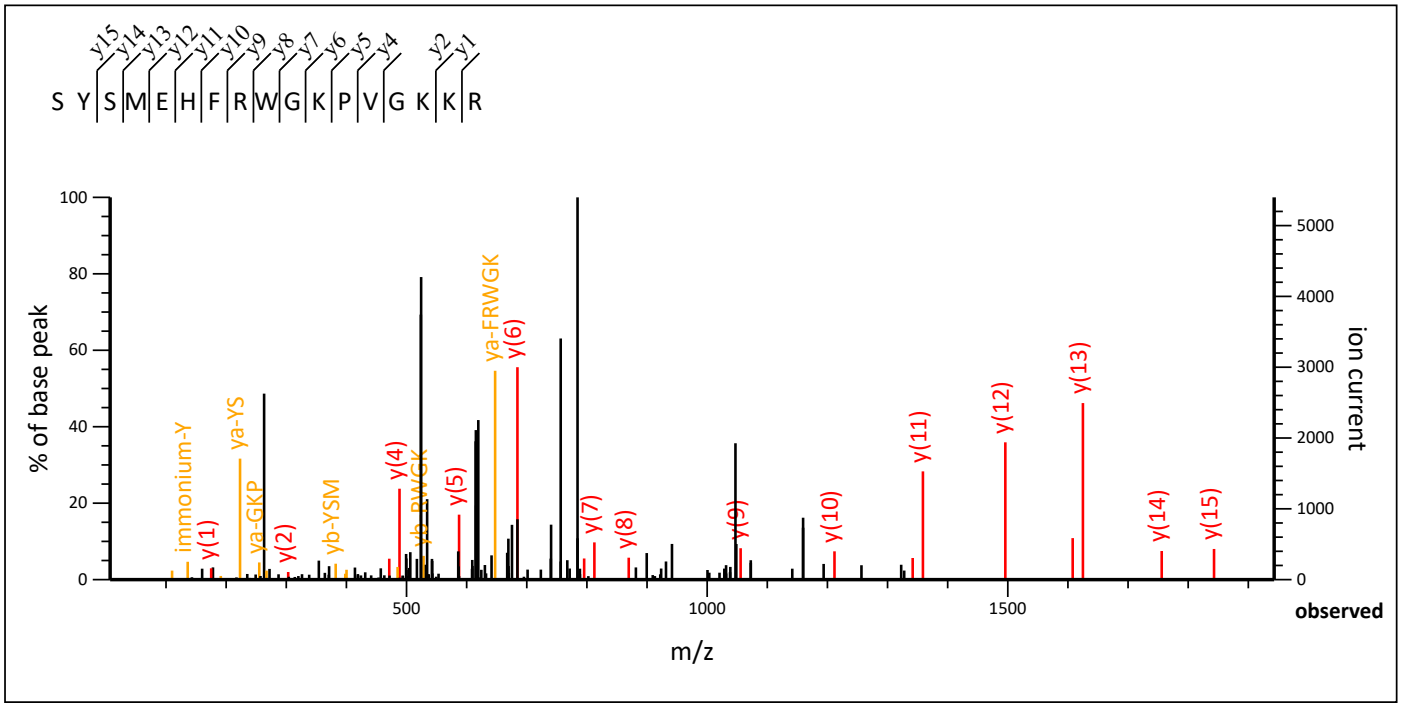
Mascot: http://www.matrixscience.com/

Mascot Search Results

Peptide View

MS/MS Fragmentation of **SYSMEHFRWGKPVGKKR**
Found in **COLI_HUMAN** in **SwissProt**, Pro-opiomelanocortin OS=Homo sapiens OX=9606 GN=POMC PE=1 SV=2

Match to Query 2: 2092.078924 from(2093.086200,1+) intensity(1.0000) index(0)
Title: Reading Top-Down experiment
Data file 524.txt



7.05 to 1943

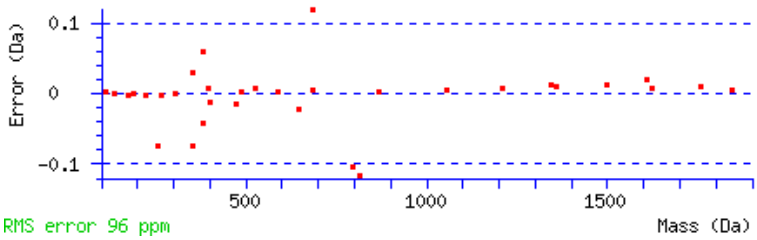
Label all possible matches ○ Label matches used for scoring ◉

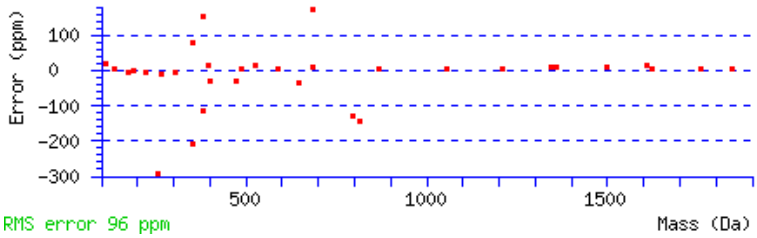
Monoisotopic mass of neutral peptide Mr(calc): 2092.0789
Ions Score: 73 **Expect:** 0.00035
Matches : 38/200 fragment ions using 73 most intense peaks (help)

#	Immon.	b	b*	b^0	Seq.	y	y*	y^0	#
1	60.0444	88.0393		70.0287	S				17
2	136.0757	251.1026		233.0921	Y	2006.0541	1989.0276	1988.0436	16
3	60.0444	338.1347		320.1241	S	*1842.9908*	1825.9643	1824.9802	15
4	104.0528	469.1751		451.1646	M	*1755.9588*	1738.9322	1737.9482	14
5	102.0550	598.2177		580.2072	E	*1624.9183*	1607.8917	1606.9077	13
6	110.0713	735.2767		717.2661	H	*1495.8757*	1478.8491		12
7	120.0808	882.3451		864.3345	F	*1358.8168*	1341.7902		11
8	129.1135	1038.4462	1021.4196	1020.4356	R	*1211.7484*	1194.7218		10
9	159.0917	1224.5255	1207.4989	1206.5149	W	*1055.6473*	1038.6207		9
10	30.0338	1281.5470	1264.5204	1263.5364	G	*869.5679*	852.5414		8
11	101.1073	1409.6419	1392.6154	1391.6314	K	*812.5465*	795.5199		7
12	70.0651	1506.6947	1489.6681	1488.6841	P	*684.4515*	667.4250		6
13	72.0808	1605.7631	1588.7365	1587.7525	V	*587.3988*	570.3722		5
14	30.0338	1662.7846	1645.7580	1644.7740	G	*488.3303*	471.3038		4
15	101.1073	1790.8795	1773.8530	1772.8690	K	431.3089	414.2823		3

16	101.1073	1918.9745	1901.9479	1900.9639	K	*303.2139*	286.1874		2
17	129.1135				R	*175.1190*	158.0924		1

Seq	ya	yb	Seq	ya	yb	Seq	ya	yb
YS	223.1077	251.1026	YSM	354.1482	382.1431	YSME	483.1908	511.1857
YSMEH	620.2497	648.2446	SM	191.0849	219.0798	SME	320.1275	348.1224
SMEH	457.1864	485.1813	SMEHF	604.2548	632.2497	ME	233.0954	261.0904
MEH	370.1544	398.1493	MEHF	517.2228	545.2177	MEHFR	673.3239	
EH	239.1139	267.1088	EHF	386.1823	414.1772	EHFR	542.2834	570.2783
HF	257.1397	285.1346	HFR	413.2408	441.2357	HFRW	599.3201	627.3150
HFRWG	656.3416	684.3365	FR	276.1819	304.1768	FRW	462.2612	490.2561
FRWG	519.2827	547.2776	FRWGK	647.3776	675.3725	RW	315.1928	343.1877
RWG	372.2142	400.2092	RWGK	500.3092	528.3041	RWGKP	597.3620	625.3569
RWGKPV	696.4304		WG	216.1131	244.1081	WGK	344.2081	372.2030
WGKP	441.2609	469.2558	WGKPV	540.3293	568.3242	WGKPVG	597.3507	625.3457
GK	158.1288	186.1237	GKP	255.1816	283.1765	GKPV	354.2500	382.2449
GKPVG	411.2714	439.2663	GKPVGK	539.3664	567.3613	GKPVGKK	667.4614	695.4563
KP	198.1601	226.1550	KPV	297.2285	325.2234	KPVG	354.2500	382.2449
KPVGK	482.3449	510.3398	KPVGKK	610.4399	638.4348	PV	169.1335	197.1285
PVG	226.1550	254.1499	PVGK	354.2500	382.2449	PVGKK	482.3449	510.3398
VG	129.1022	157.0972	VGK	257.1972	285.1921	VGKK	385.2922	413.2871
GKK	286.2238	314.2187	KK	229.2023	257.1972			





NCBI **BLAST** search of SYSMEHFRWGKPVGKKR
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc)	Delta	Sequence
73.0	2092.0789	0.0001	SYSMEHFRWGKPVGKKR
8.7	2092.0589	0.0200	DEVLDAQQRGVFGQVLTAF
7.2	2092.0986	-0.0197	QQLDGAAALYKLANKSMALS
6.8	2092.0663	0.0126	IHSCIISPSLTEAHVEPLF
6.6	2092.0966	-0.0177	LRKAENIGNRYHFNIFT
6.4	2092.0986	-0.0197	QGTLAGRSPISIAASGIYMIS
5.6	2092.0962	-0.0172	MLLGKPLFKGHDHLDQLM
5.3	2092.0623	0.0167	SALQAALSASGAIFQTAKPGTC

5.2	2092.0773	0.0016	SGIPRSSQELDRRSSVYR
5.0	2092.0629	0.0160	SSYFLHLHSSSFLLLPASS

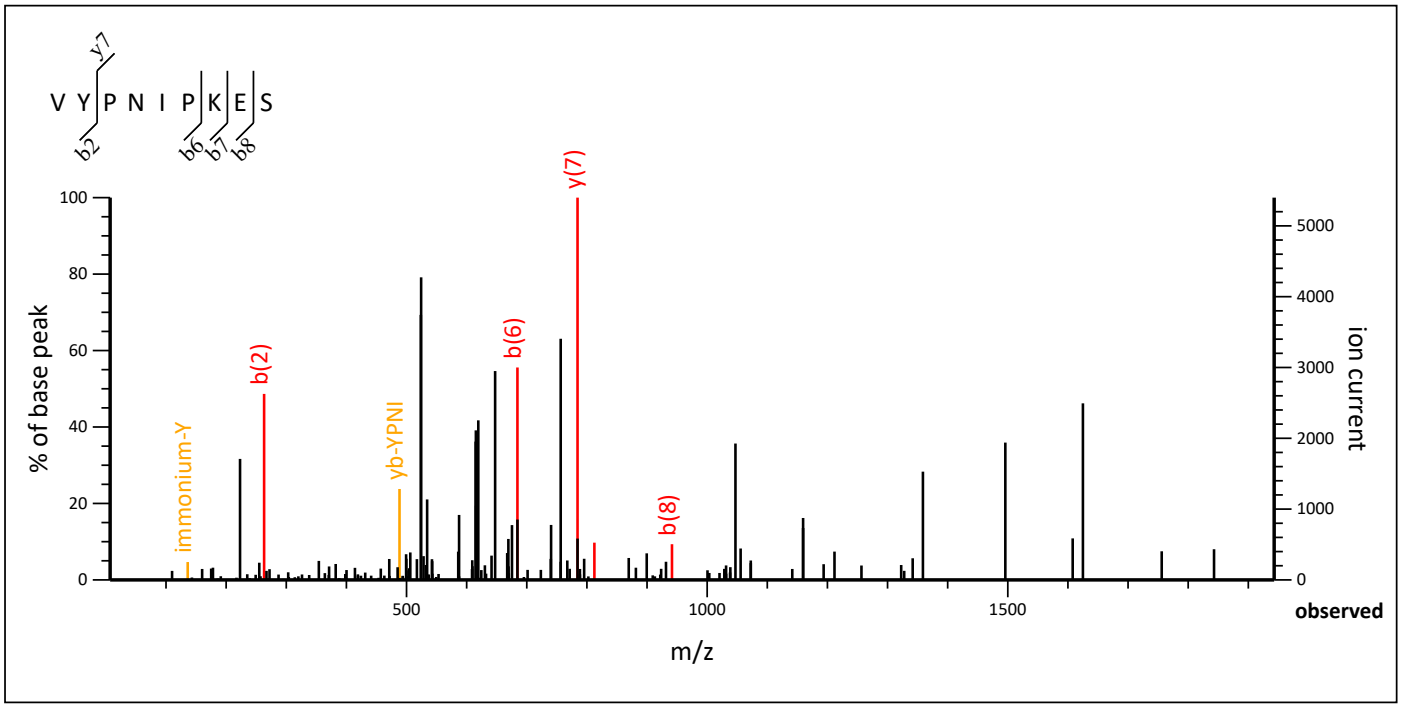
Mascot: http://www.matrixscience.com/

Mascot Search Results

Peptide View

MS/MS Fragmentation of **VYPNIPKES**
Found in **FMO3_BOVIN** in **SwissProt**, Dimethylaniline monooxygenase [N-oxide-forming] 3 OS=Bos taurus OX=9913 GN=FMO3 PE=2 SV=1

Match to Query 1: 1045.534524 from(1046.541800,1+) intensity(1.0000) index(0)
Title: Reading Top-Down experiment
Data file 524.txt



7.05 to 1943

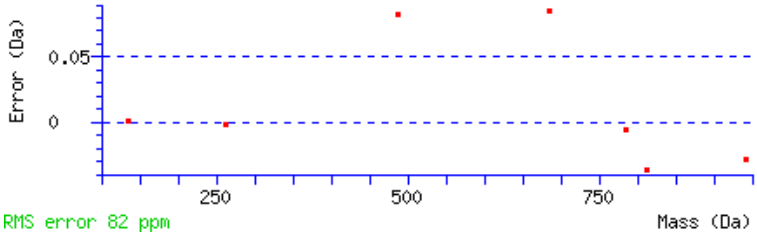
Label all possible matches ○ Label matches used for scoring ◉

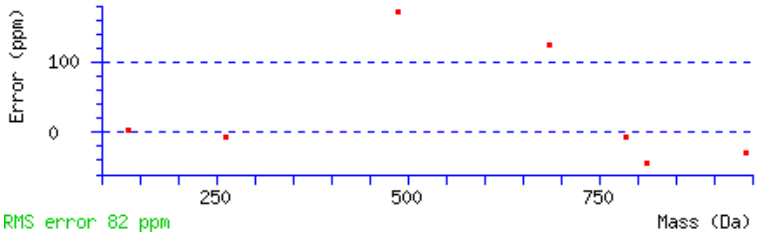
Monoisotopic mass of neutral peptide Mr(calc): 1045.5444
Ions Score: 25 **Expect:** 20
Matches : 7/84 fragment ions using 10 most intense peaks (help)

#	Immon.	b	b*	b^0	Seq.	y	y*	y^0	#
1	72.0808	100.0757			V				9
2	136.0757	***263.1390***			Y	947.4833	930.4567	929.4727	8
3	70.0651	360.1918			P	**784.4199**	767.3934	766.4094	7
4	87.0553	474.2347	457.2082		N	687.3672	670.3406	669.3566	6
5	86.0964	587.3188	570.2922		I	573.3243	556.2977	555.3137	5
6	70.0651	***684.3715***	667.3450		P	460.2402	443.2136	442.2296	4
7	101.1073	***812.4665***	795.4400		K	363.1874	346.1609	345.1769	3
8	102.0550	***941.5091***	924.4825	923.4985	E	235.0925		217.0819	2
9	60.0444				S	106.0499		88.0393	1

Seq	ya	yb	Seq	ya	yb	Seq	ya	yb
YP	233.1285	261.1234	YPN	347.1714	375.1663	YPNI	460.2554	488.2504
YPNIP	557.3082	585.3031	YPNIPK	685.4032		PN	184.1081	212.1030
PNI	297.1921	325.1870	PNIP	394.2449	422.2398	PNIPK	522.3398	550.3348

PNIPKE	651.3824	679.3774	**NI**	200.1394	228.1343	**NIP**	297.1921	325.1870
NIPK	425.2871	453.2820	**NIPKE**	554.3297	582.3246	**IP**	183.1492	211.1441
IPK	311.2442	339.2391	**IPKE**	440.2867	468.2817	**PK**	198.1601	226.1550
PKE	327.2027	355.1976	**KE**	230.1499	258.1448			





NCBI **BLAST** search of VYPNIPKES
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc)	Delta	Sequence
24.9	1045.5444	-0.0099	VYPNIPKES
24.9	1045.5444	-0.0099	VYPNLPKES
23.1	1045.5345	0.0000	DRVYIHPF
16.2	1045.5305	0.0040	FDSRHLKGS
14.3	1045.5404	-0.0058	KGVEAAQSKE
11.8	1045.5291	0.0054	GKLTAALEDE
11.2	1045.5345	0.0000	DRIYVHPF
11.0	1045.5404	-0.0059	LGTKVERDE
11.0	1045.5404	-0.0059	LTGKVREDE
10.9	1045.5305	0.0040	YVRHQKDT

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